

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 4120 mmHg

Global applicability domain: Inside

Local applicability domain index: 5.48e-01

Confidence level: 6.92e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Cyclohexane, 1,1,2,2,3,3,4,4,5,5,6- undecafluoro-6-(trifluoromethyl)- Measured: 2010 Predicted: 107</div>	<div>Image not found</div> <div>Dalapon Measured: 6630 Predicted: 2.61e-01</div>	<div>Image not found</div> <div>Chloropentafluoroethane Measured: 25100 Predicted: 6690</div>
<div>Image not found</div> <div>Carbonic difluoride Measured: 2000 Predicted: 20100</div>	<div>Image not found</div> <div>Fluoroacetone Measured: 3410 Predicted: 143</div>	